

Modelling Homogenisation Heat Treatment

Homogenisation heat treatment is a critical stage in the processing of cast alloys. It is performed with the goal of improving mechanical properties through the removal of microsegregation within the primary matrix phase, dissolution of undesirable secondary phases, and growth of suitable ones depending on temperature and alloy chemistry.^[1-3] The use of effective modelling tools can reduce costs and optimise the design of homogenisation schedules, which is often done empirically on a trial and error basis. This report provides an overview of the approach used in JMatPro® v12 to model the homogenisation of as-cast structures, which builds on previous versions^[1] to deal with the growth or dissolution of secondary phases simultaneously with the removal of microsegregation in the matrix.

Model Description

The first part of the model requires building a microsegregation profile, which shows how the solute concentration varies within a characteristic distance in the alloy's microstructure, usually taken as half of the secondary dendrite arm spacing, λ . In JMatPro® this may be accomplished after performing a solidification calculation using either the classical Scheil-Gulliver model^[4] or its extension to include the effect of back diffusion in the primary solid phase.^[5] If back diffusion is considered, the solute concentration profiles are a direct result of the calculation, while in the Scheil-Gulliver case they are obtained by establishing a correlation between the fraction of solid formed, f_s , and a position along the dendrite, r ,

$$f_s = \left(\frac{r}{\lambda}\right)^{g+1} \quad (1)$$

where the coefficient $g = 0,1,2$ is used to describe three possible dendrite geometries: plate, cylinder, or sphere, respectively.

In addition to the primary matrix phase, several nonequilibrium secondary phases may exist after solidification and dissolve during the homogenisation heat treatment. Depending on temperature and alloy chemistry, the growth of equilibrium phases may also be possible during homogenisation. For multicomponent alloys, the actual case may be quite complex and thus simplified assumptions are required. In the model this is dealt with by treating each component independently and introducing the concept of pseudo-eutectic,^[1] which gathers the various phases that will either dissolve or grow during homogenisation in a single structure. The pseudo-eutectic and its fate are established following the steps below:

1. First, an equilibrium calculation is performed at the homogenisation temperature, T_h . The total amount of solute component i in the primary solid phase at equilibrium, $S_{eq,i}$, is then compared with the corresponding amount at the end of solidification, $S_{std,i}$.
2. If $S_{eq,i} > S_{std,i}$, the pseudo-eutectic is added to the concentration profile, in effect creating a source of extra solute that will dissolve into the matrix during homogenisation. The concentration of solute component i in the pseudo-eutectic, $C_{pe,i}$, is taken as that of the remaining liquid, while its fraction, $f_{pe,i}$, is calculated as:^[1]

$$f_{pe,i} = \frac{S_{eq,i} - S_{std,i}}{C_{pe,i}} \quad (2)$$

3. If $S_{eq,i} < S_{std,i}$, the concentration profile at the end of solidification remains unchanged and the extra solute is removed from the matrix by growing an additional fraction of pseudo-eutectic during homogenisation. In this case, the fraction of pseudo-eutectic that may ultimately form is taken as the sum of all secondary phase fractions containing component i at equilibrium, subtracted from those of nonequilibrium phases left at the end of solidification. The concentration is given by:

$$C_{pe,i} = \frac{S_{std,i} - S_{eq,i}}{f_{pe,i}} \quad (3)$$

The simulation of the homogenisation process consists of two stages. In the first stage, the pseudo-eutectic either dissolves or grows and, in the subsequent stage, the microsegregation in the matrix is removed. Throughout the calculation, solute diffusion is only considered explicitly in the matrix phase. The evolution of the concentration profile for component i in the matrix, $C_{mat,i}(r)$, is governed by Fick's second law,^[6,7]

$$\frac{\partial C_{mat,i}}{\partial t} = D_i \left(\frac{\partial^2 C_{mat,i}}{\partial r^2} + \frac{g}{r} \frac{\partial C_{mat,i}}{\partial r} \right) \quad (4)$$

with the diffusion coefficients given by:^[6]

$$D_i = D_i^0 \exp \left(-\frac{Q_i}{RT_h} \right) \quad (5)$$

where D_i^0 denotes a frequency factor, Q_i a molar activation energy, and $R = 8.3144 \text{ J mol}^{-1} \text{ K}^{-1}$ is the gas constant.

The difference between the two stages is expressed in the boundary conditions used towards the edge of the dendrite. In the first stage, the concentration in the matrix at the interface with the pseudo-eutectic remains fixed at the value obtained at the end of solidification (or the equilibrium value, whichever is more appropriate). At each time step, the interface is displaced by requiring conservation of solute:

$$(1 - f_{pe,i})C_{mat,i} + f_{pe,i}C_{pe,i} = const \quad (6)$$

The first stage proceeds until the fraction of pseudo-eutectic becomes zero (in the case of dissolution) or reaches its maximum value as explained above (in the case of growth). Afterwards, the second stage begins, and a zero-flux boundary condition is imposed:

$$\frac{\partial C_{mat,i}}{\partial r} = 0 \quad (7)$$

The above condition is also used at the centre of the dendrite for both stages.

Note that the evolution of the pseudo-eutectic is fully dictated by solute diffusion and mass balance, hence the time required for dissolution or growth comes out naturally from the calculation. If the concentration profile flattens out too quickly, it is possible that the pseudo-eutectic will not completely dissolve or reach the predicted maximum growth. The same is expected for slow diffusing solutes or low homogenisation temperatures.

Case Studies

Figure 1 shows the concentration profiles calculated for alloy AA356 (Al-0.4Mg-7Si wt%) following different homogenisation heat treatment times at 540 °C. The initial as-cast profiles were obtained after a

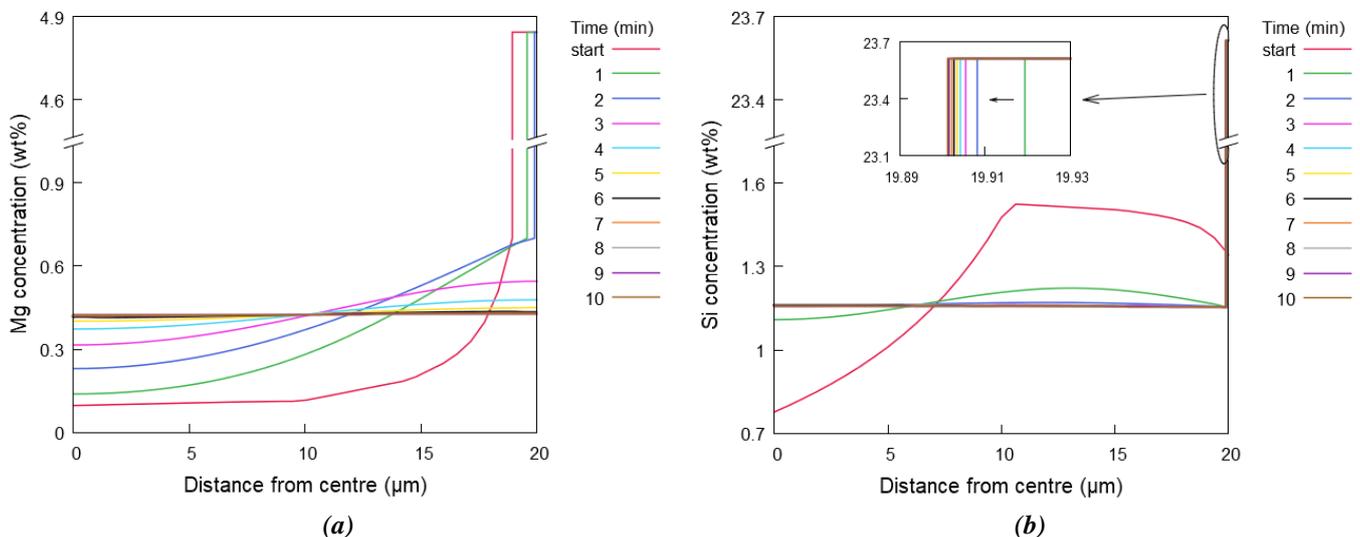


Figure 1: Calculated concentration profiles of Mg (a) and Si (b) after homogenisation of alloy AA356 at 540 °C for different times. Inset shows how the pseudo-eutectic is growing at the edge of the dendrite for Si.

solidification calculation using the Scheil-Gulliver model, and a plate dendrite geometry was assumed with the secondary dendrite arm spacing set to the experimental value of 40 μm .^[2] As can be seen in Fig. 1(a), the pseudo-eutectic dissolves for Mg and is no longer present after only 3 minutes. This corresponds to the dissolution process of Mg_2Si particles observed in the homogenisation treatment of real castings.^[2,3] The calculated dissolution time agrees very well with the experimental value of 2–4 minutes.^[2] For Si, on the other hand, the pseudo-eutectic grows during homogenisation [see Fig. 1(b)], which corresponds to the coarsening of eutectic Si particles.^[3] The growth is largely complete after 3 minutes, when the Si concentration in the matrix is already rather flat. In the homogenisation of real castings, this typically proceeds for much longer.^[3] A more complex treatment of coarsening would be required to capture this accurately in the model. It is reasonable to assume that the removal of microsegregation in the matrix is controlled by the slowest diffusing element, in this case Mg. Setting the criterion for complete homogenisation as a solute fluctuation of no more than 0.01 wt%, a homogenisation time of 8 minutes is obtained. This is in line with experimental values of about 8–15 minutes.^[2]

Figure 2 shows the concentration profiles obtained for alloy AA357 (Al-0.62Mg-7Si wt%) after homogenisation heat treatment at 540 °C for various times. As before, the as-cast profiles were derived from a Scheil-Gulliver calculation, and a plate dendrite geometry was considered only with a larger secondary dendrite arm spacing (the experimental value of 55 μm ^[2] was used). As can be seen by comparing Figs. 1 and 2, the initial segregation is similar to that of alloy AA356, but the increased diffusion length leads to considerably longer dissolution and homogenisation times. For Mg the pseudo-eutectic dissolves after about 10 minutes and it takes around 18 minutes to reach homogenisation [see Fig. 2(a)]. For Si the pseudo-eutectic reaches its maximum growth within 2 to 4 minutes, similar to the case of alloy AA356, while the time required to obtain a homogenised matrix profile increases to about 8 minutes. These results agree with the trend observed experimentally, with the reported dissolution and homogenisation times increasing to <50 minutes as the Mg content is increased from 0.4 to 0.62 wt%.^[2]

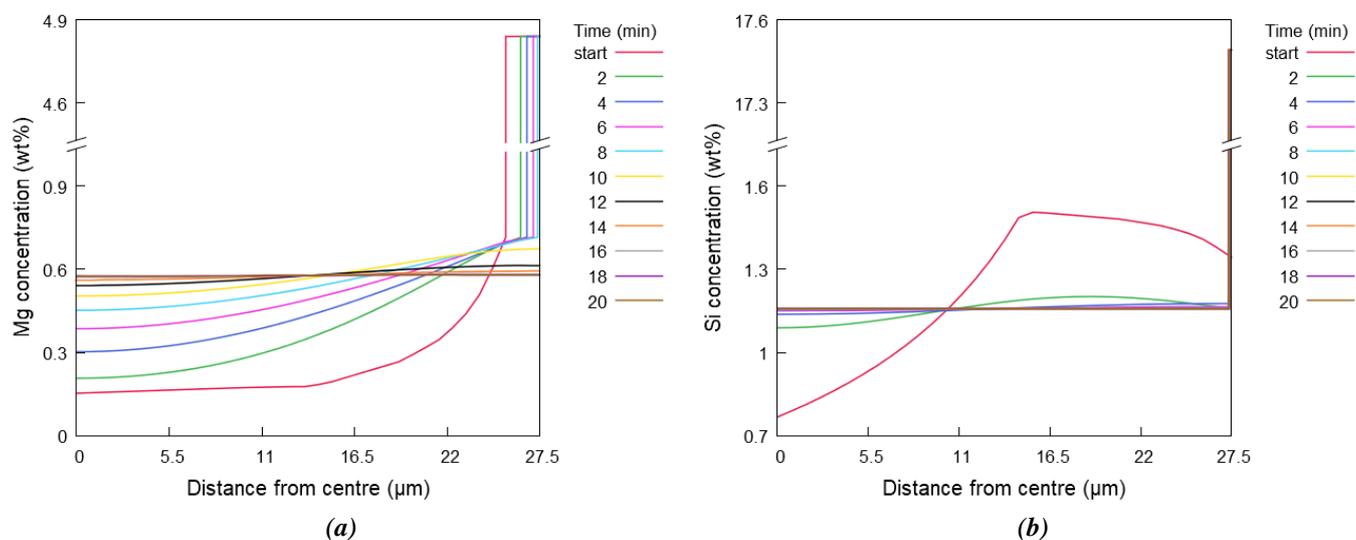


Figure 2: Calculated concentration profiles of Mg (a) and Si (b) after homogenisation of alloy AA357 at 540 °C for different times.

Summary

The model used in JMatPro® v12 to simulate the homogenisation heat treatment of as-cast structures has been described. It extends the concept of pseudo-eutectic of previous versions to allow for a simple and unified treatment of the growth or dissolution of secondary phases simultaneously with the removal of microsegregation in the matrix.

It has been shown that this approach is sufficiently robust to predict time scales and trends observed experimentally. As such, it can be a useful tool to aid in the design of homogenisation heat treatment schedules for the processing of industrial cast alloys.

References

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